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# Self-Diffusion in Liquid Copper, Silver, and Gold

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**Abstract:** The recently developed by us semi-analytical representation of the mean spherical approximation in conjunction with the linear trajectory approximation is applied to the quantitative study of self-diffusivities in liquid Cu, Ag and Au at different temperatures. The square-well model is employed for the description of the interatomic pair interactions in metals under study. It is found that our theoretical results are in good agreement with available experimental and computer-simulation data and can be considered as a prediction when such data are absent.

**Keywords:** liquid metal; diffusion; square-well model; mean spherical approximation; linear trajectory approximation

## 1. Introduction

An experimental study of diffusion properties in metal melts is a hard task. Progress in this field is connected with the arising of new techniques in the last two decades [1–20]. In particular, modern precise measurements provided a finding that small additions in dilute germanium weakly affect its diffusion coefficients in spite of the very big difference between their atomic mass [20]. Nevertheless, despite big progress spreading to binary and multicomponent alloys, the discrepancy in experimental results remains up to the present time, even for pure liquid metals. Therefore, theoretical approaches serve as an efficient instrument for investigations in this area. One of them is the square-well (SW) model, which is actively applied to liquid metals and their alloys [21–29].

In the last years, the square-well model and closely related to its models are intensively developed, including its applications to diffusivities' calculations [30–40]. Some years ago, we introduced the semi-analytical method [41] of solving the Ornstein–Zernike equation [42] for the SW model within the mean spherical approximation (MSA) [43]. Then, this method, in conjunction with the linear trajectory approximation (LTA) [44,45], was successfully used to calculate the self-diffusion coefficients of liquid alkali metals and their binary mixtures [46–48].

Here, we apply the aforementioned SW-MSA-LTA approach for the quantitative study of self-diffusivities in liquid noble metals and compare obtained results with available experimental and computer-simulation data.

## 2. Theory

In the majority of model theories, the Einstein relation is the basis for calculating the self-diffusion coefficient, $D$, of the atom in the pure liquid as a quantity which is inversely proportional to the friction coefficient, $\xi$, of the same atom [49]:

$$D = (\beta\xi)^{-1} \quad (1)$$

where $\beta = (k_B T)^{-1}$; $k_B$ is the Boltzmann constant; $T$ is the temperature.

In the theory of liquids, there are many ways to determine $\xi$ [50,51]. Among them, the linear trajectory approximation is one of the best. It was introduced by Helfand [44] for fluids described by any hard-core (HC) pair potential, $\phi_{\mathrm{HC}}(r)$, to take into account the non-hard-core contribution to the friction coefficient, $\xi_{\mathrm{non-HC}}$:

$$\xi_{\mathrm{non-HC}} = -\frac{(\beta\pi M)^{1/2}}{12\pi^2}\int_0^\infty [S(q)-1]\varphi_{\mathrm{HC}}(q)\, q^3 \mathrm{d}q \tag{2}$$

Here, $M$ is the atomic mass; $S(q)$ is the structure factor in the corresponding HC model; $\varphi_{\mathrm{HC}}(q)$ is the Fourier transform of $\phi_{\mathrm{HC}}(r)$ outside the hard core, $\varphi_{\mathrm{HC}}(r)$:

$$\varphi_{\mathrm{HC}}(q) = 4\pi\int_\sigma^\infty \varphi_{\mathrm{HC}}(r)\frac{\sin(qr)}{qr} r^2 \mathrm{d}r \tag{3}$$

Together with the contribution from the hard-core part of the pair interaction, $\xi_{\mathrm{HC}}$, suggested earlier in [52] the contribution $\xi_{\mathrm{non-HC}}$ allows to write the total friction coefficient for pure liquids in the framework of the Helfand theory:

$$\xi = \xi_{\mathrm{HC}} + \xi_{\mathrm{non-HC}} \tag{4}$$

where

$$\xi_{\mathrm{HC}} = \frac{8}{3}\rho\sigma^2 g(\sigma)\,(\pi M/\beta)^{1/2} \tag{5}$$

$\rho$ is the mean atomic density, $\sigma$ is the diameter of the hard core, $g(r)$ is the pair correlation function of the HC model under consideration.

Davis and Palyvos [45] modified Equation (4) by taking into account the cross effect between HC and non-HC forces:

$$\xi = \xi_{\mathrm{HC}} + \xi_{\mathrm{non-HC}} + \xi_{\mathrm{cross}} \tag{6}$$

where

$$\xi_{\mathrm{cross}} = -\tfrac{1}{3}\rho\,(\beta M/\pi)^{1/2} g(\sigma)\int_0^\infty [x\cos(x)-\sin(x)]\,\varphi_{\mathrm{HC}}(q)\,\mathrm{d}q\,, \quad x = q\sigma \tag{7}$$

As a hard-core potential, we take the square-well one:

$$\phi_{\mathrm{SW}}(r) = \begin{cases} \infty, & r < \sigma \\ \varepsilon, & \sigma \le r < \lambda\sigma \\ 0, & r \ge \lambda\sigma \end{cases} \tag{8}$$

where $\varepsilon$ and $\sigma(\lambda-1)$ are the depth and the width of the square well, respectively.

The Fourier transform (3) of its non-hard-core part leads to:

$$\phi_{\mathrm{SW}}(q) = 4\pi\varepsilon\,[\sin(\lambda x)-\sin(x)-\lambda x\cos(\lambda x)+x\cos(x)]\,/q^3 \tag{9}$$

For the SW potential, Equations (2), (5) and (7) are being rewritten, respectively, as:

$$\xi_{\mathrm{non-HC}} = -\frac{(\beta\pi M)^{1/2}}{12\pi^2}\int_0^\infty [S_{\mathrm{SW}}(q)-1]\phi_{\mathrm{SW}}(q)\, q^3 \mathrm{d}q \tag{10}$$

$$\xi_{\mathrm{HC}} = \frac{8}{3}\rho\sigma^2 g_{\mathrm{SW}}(\sigma)\,(\pi M/\beta)^{1/2} \tag{11}$$

$$\xi_{\text{cross}} = -\frac{1}{3}\rho\,(\beta M/\pi)^{1/2} g_{\text{SW}}(\sigma) \int_0^\infty [x\cos(x) - \sin(x)]\,\varphi_{\text{SW}}(q)\,\mathrm{d}q \tag{12}$$

where

$$S_{\text{SW}}(q) = \frac{1}{1 - \rho c_{\text{SW}}(q)} \tag{13}$$

Here, $c_{\text{SW}}(q)$ is the Fourier transform of the SW partial direct correlation function, $c_{\text{SW}}(r)$. The calculation of $c_{\text{SW}}(q)$ is not a trivial task as it is for the analogous function within the hard-sphere model for which the analytical solution is known [53,54]. In our work, $c_{\text{SW}}(r)$ is represented in the semi-analytical form of the mean spherical approximation [41,47]:

$$c_{\text{SW}}(r) = \begin{cases} \sum\limits_{m=0}^{n} b_m \left(\frac{r}{\sigma}\right)^m, & r < \sigma \\ -\beta\varphi_{\text{SW}}(r), & r \geq \sigma \end{cases} \tag{14}$$

where $n \geq 3$; $b_m$ are the coefficients determined during fulfilling the condition that the pair correlation function must be equal to zero inside the hard core:

$$g_{\text{SW}}(r) = 0 \text{ at } r < \sigma \tag{15}$$

The Fourier transform of Equation (14),

$$c(q) = 4\pi \int_0^\infty c(r) \frac{\sin(qr)}{qr} r^2 \mathrm{d}r \tag{16}$$

gives

$$c_{\text{sw}}(q) = -\beta\varphi_{\text{sw}}(q) + \left(\frac{4\pi}{q^3}\right)\left\{\sum_{m=1}^{n+2} x^{2-m} \frac{\partial^m \sin(x)}{\partial x^m} \sum_{l=0}^{n} b_l \prod_{k=0}^{m-2}(l+1-k) + \sum_{m=1}^{[(n+1)/2]} \frac{(-1)^{m+1}(2m)!\,b_{(2m-1)}}{x^{2m-1}}\right\} \tag{17}$$

where $[(n+1)/2]$ is the integral part of $(n+1)/2$.

To numerically solve Equation (15), we use the simplex method in conjunction with the Fourier transform of $g_{\text{SW}}(r)$,

$$g_{\text{SW}}(r) = 1 + \frac{1}{2\pi^2\rho} \int_0^\infty [S_{\text{SW}}(q) - 1] \frac{\sin(qr)}{qr}\, q^2 \mathrm{d}q \tag{18}$$

at $n = 5$.

## 3. Results and Discussion

The calculations are fulfilled at temperatures at which the experimental information about the mean atomic densities and structure factors of liquid metals under consideration is available [55]. The corresponding values of $T$ and $\rho$ are listed in Table 1. Experimental $S(q)$ are needed to find adjustable values of the SW parameters by fitting the calculated structure factor with respect to the experimental one at each temperature.

**Table 1.** Input values of $\rho$ (kg/m$^3$) used for calculations.

| Metal | $T$ = 1273 K | $T$ = 1423 K | $T$ = 1573 K | $T$ = 1773 K | $T$ = 1873 K |
|---|---|---|---|---|---|
| Cu | - | 7970 | 7860 | 7690 | 7620 |
| Ag | 9270 | 9120 | 8980 | - | - |
| Au | - | 17,200 | 17,100 | 16,900 | - |

The obtained results are represented in Figures 1–3, together with experimental, classical molecular dynamics (MD), and ab initio MD results available in the literature.

For liquid Cu (Figure 1), there are two experimental works on the self-diffusion coefficient [6,56]. Our results, as well as the ab initio MD [57,58] and classical MD [59–61] results, agree significantly better with the modern experiment of Meyer [6] rather than with one of Henderson and Yang [56] while the classical MD results of Mei and Davenport [62] are approximately equidistant from both experimental series. Note that other classical MD calculations [63,64] give essentially higher values of $D$ even in comparison with the results of [56].

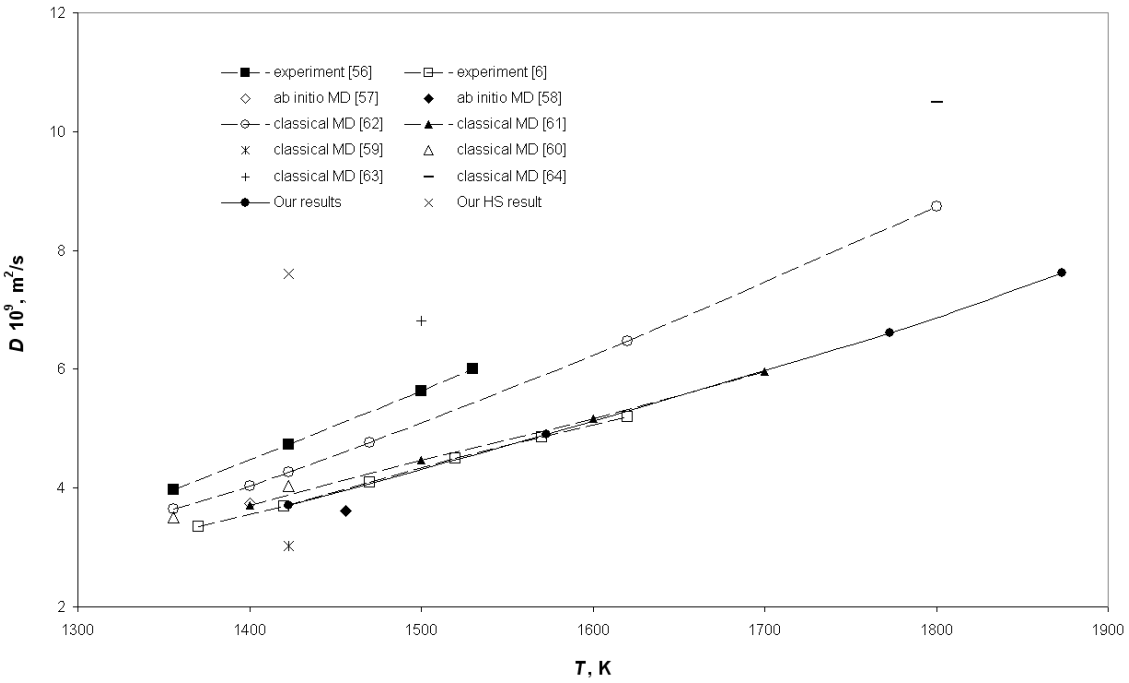


**Figure 1.** Self-diffusion coefficient of liquid Cu.

Our values of $D$ for liquid Ag are lower than ones from all three experimental works [1,14,65]. However, the tendency to convergence with experimental data with an increase in the temperature is observed (Figure 2). A better agreement (deviation is less than 15%) is observed with more recent experimental results [14]. There is also good agreement with results [65] (which are extrapolated to different from available in the original work temperatures using the empirical relation from [51]). The accuracy of the experiment of Itami et al. [1] is not completely reliable to our opinion since the temperature dependence of the self-diffusion coefficient in [1] has the minimum at some temperature.

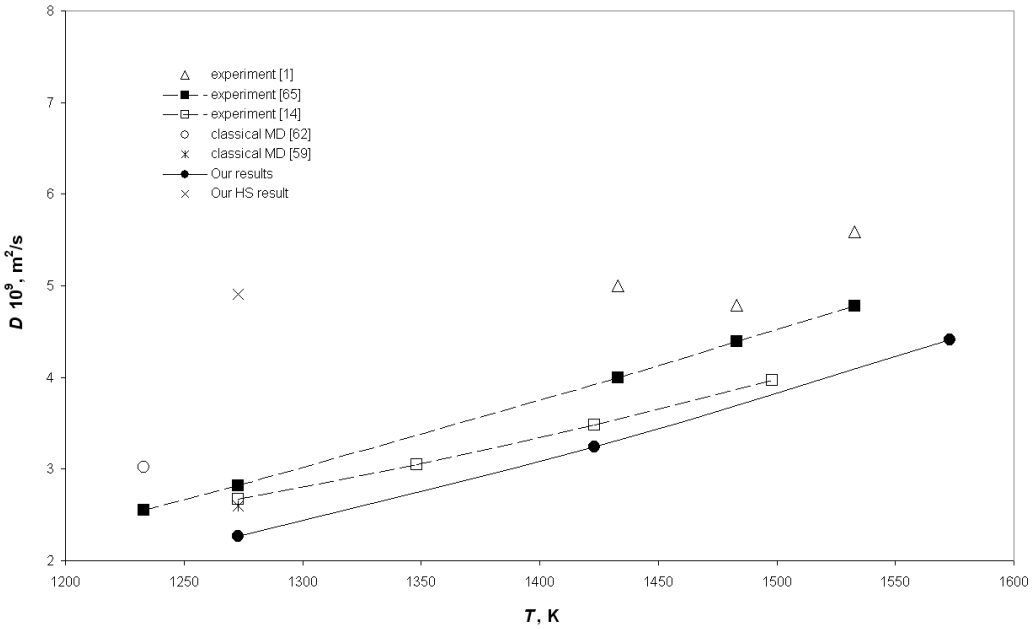


**Figure 2.** Self-diffusion coefficient of liquid Ag.

For liquid Au (Figure 3), the experimental results on the self-diffusion coefficient are not available. There are two ab initio [66,67] and three classical [59,62,68] MD simulations at different temperatures. The discrepancy between these results is very big. For example, the result of the work [62] obtained $T = 1336$ K is approximately three times bigger than the corresponding value of $D$ which can be approximated from Figure 3 of the work [66] at the same temperature. On the whole, the classical MD simulations (except for [59]) give significantly higher values $D$ than ab initio MD simulations. Our result lies very close to the ab initio MD results of Peng et al. [67], which are approximately average between the ab initio MD results of [66] and the classical MD result of [59].

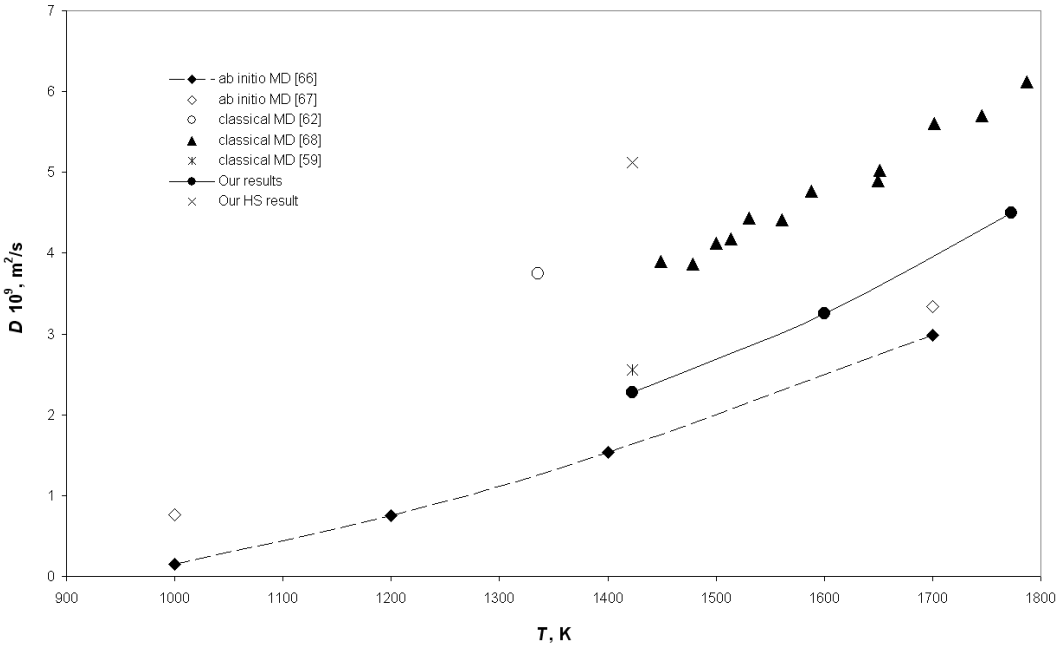


**Figure 3.** Self-diffusion coefficient of liquid Au.

Additionally, we calculated $D$ within the hard-sphere (HS) model at the lowest among taken for each metal temperature (Figures 1–3).It is clear that the HS results are sufficiently crude.

## 4. Conclusions

In the present work, it is found that the semi-analytical representation of the mean spherical approximation applied to the square-well model in the frameworks of the linear trajectory approximation allows obtaining good quantitative results for the self-diffusivities in liquid noble metals. Moreover, as well as for alkali liquid metals and their alloys [46–48], this good description is achieved with the SW-parameters' values defined from the structure data that shows the universality of the used approach.

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**Conflicts of Interest:** The author declares no conflict of interest.

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